Mangalore University

Department of Studies in Chemistry

M. Sc. Degree Programme

(CHOICE BASED CREDIT SYSTEM - SEMESTER SCHEME)

Syllabi for M.Sc., Courses in

ANALYTICAL CHEMISTRY

(From the Academic Year 2016-17 onwards)

Mangalore University

M. Sc. Degree Programme in Analytical Chemistry:

CHOICE BASED CREDIT SYSTEM (CBCS) SEMESTER SCHEME

C O U R S E P A T T E R N AND S C H E M E OF E X A M I N A T I O N

(Year 2016-2017 onwards)

PREAMBLE

Revision of Syllabi for the Two years Master Degree (Choice Based Credit System-Semester Scheme) Pogrammes in Chemistry, Applied Chemistry, Organic Chemistry and Analytical Chemistry.

PG BOS in Chemistry has revised and prepared the Syllabi (CBCS based) for all the Four Courses -Chemistry, Applied Chemistry, Organic Chemistry and Analytical Chemistry in its meeting held on 24th July 2014 and the University implemented it from the same academic year. Now the University has asked the PG BOS in Chemistry to revise the syllabi by giving certain Guidelines (Ref:-No: MU/ACC/CR.38/ CBCS (PG)/2015-16 dt.05-05-2016 bse on UGC letter) for all the four Courses (Programmes) to offer Hard Core, Soft Core and Open Elective course papers with credits to each course amounting to 92 credits for the entire programme.

Accordingly, the PG BOS in Chemistry prepared the syllabi for all the four programmes. It has prepared course pattern by proposing 12 Hard Core theory courses (3 in each semester) and 5 practical courses (in 3rd and 4th semester), one Project work (in 4th Semester with 4 credits)with a provision to have One Project Work in lieu of one of the practicals in 4th semester in each programme with 3 credits each(project work - 4 credits) with total of **55 Credits**). BOS is offering 3, 2, 2 and 3 (Total 10 courses) Soft core courses respectively in 1st , 2nd, 3rd and 4th semesters of a programme. Student shall opt any 2, 1, 1 and 2(Total 6 courses) courses respectively in 1st , 2nd , 3rd, 4th Semesters. All the soft core papers are of 3 credits. Programma consists of 6 Soft Core practical courses (3 courses each in 1st and 2nd semesters of the Programme with 2 credits each) with a total of **30 credits** (6 theory x 3 credits + 6 practicals x 2 credits). BOS has also proposed 2 open electives (1 each in 2nd& 3rd Semesters of the programme) with 3 credits each (**6 credits)**. All together **total credits** come to 91from teaching. I have prepared a draft course pattern by considering all the points mentioned in the above said letter from the Registrar and placing it before the BOS meeting.

Detailed syllabi for 1st and 2nd Semesters are prepared and enclosed, whereas the syllabi for the 3rd and 4th Semesters will be prepared in forthcoming BOS meeting.

Course/credit pattern:

Semester Credits	Hard Core(H)(T)	Soft Core (S)(T)	Elective E)(T)	Practical	Tutorial	Total Credits
First	9	6	--	6 (S)	--	21
Second	9	3	3	6 (S)	--	21
Third	9	3	3	9 (H)	--	24
Fourth	9	6	--	10(H)	--	25
Total	36	18	6*	12(S) + 19(H)	--	91

Total Credits from all the Four Semesters (1^{st} , 2^{nd} , 3^{rd} and 4^{th}) : 21+21+24+25 = 91

Total Hard Core credits = 36 (T) + 19 (P) = 55 = 60.4%

Total Soft Core credits = 18 (T) + 12(P) = 30 = 33.0%

*Open Elective Credits = 6 = 6.6% (Not to considered for calculating the CGPA)

H= Hard Core, S= Soft Core, P =Pratical/Project

Programme : M.Sc in Analytical Chemistry

1st Semester **2nd Semester**

Course Code	Course Title	Course Code	Course Title
CA H 401	Inorganic Chemistry	CA H 451	Advanced Inorganic Chemistry
CA H 402	Organic Chemistry	CA H 452	Advanced Organic Chemistry
CA H 403	Physical Chemistry	CA H 453	Advanced Physical Chemistry
CAS 404 Or CA S 405	Inorganic Spectroscopy and Analytical Techniques Or Environmental Chemistry	CA S 454 CA S 455	Organic Spectroscopic Techniques Or Chemistry of Bio-molecules
CA S 406	Molecular Spectroscoy and Diffraction Techniques	CA E 456	Environmental, Electro- and Surface Chemistry
CA P 407	Inorganic Chemistry Practicals-1	CA P 457	Inorganic Chemistry Practicals-II
CA P 408	Organic Chemistry Practicals-1	CA P 458	Organic Chemistry Practicals-II
CA P 409	Physical Chemistry Practicals-1	CA P 459	Physical Chemistry Practicals-II

3rd Semester **4th Semester**

CA H 501	Principles of Analytical Chemistry	CA H 551	Applied Analysis
CA H 502	Bioanalytical & Radiochemical Techniques	CA H 552	Optical Methods of Analysis
CA H 503	Chromatographic Separation Techniques	CA H 553	Process Analytical Chemistry
CA S 504 Or CA S 505	Thermoanalytical Techniques Or Analytical Chemistry of Polymers	CA H 554 Or CA S 555	Environmental Chemistry Or Pharmacokinetics & Nanimaterials
CA E 506	Analytical and Green Chemistry	CA S 555	Separation Techniques
CA P 507	Analytical Chemistry Practicals-III	CA P 557	Analytical Chemistry Practicals-VI
CA P 508	Analytical Chemistry Practicals -IV	AC P 558	Analytical Chemistry Practicals-VII
CA P 509	Analytical Chemistry Practicals -V	CA P 559	Project Work & Dissertation

Detailed distribution of Course &Credits:

Programme: **Analytical Chemistry :**

1st Semester

Course Code	Course Title	No of Units	Evaluation IA + Exam	Teaching hrs week	Sem	Exam hrs	Credits
CA H 401	Inorganic Chemistry	3	30 + 70	3	45	3	3
CA H 402	Organic Chemistry	3	30 + 70	3	45	3	3
CA H 403	Physical Chemistry	3	30 + 70	3	45	3	3
CAS 404 Or CA S 405	Inorganic Spectroscopy and Analytical Techniques Or Environmental Chemistry	3 3	30 + 70 30 + 70	3 3	36 36	3	3
CA S 406	Molecular Spectroscoy and Diffraction Techniques	3	30 + 70	3	36	3	3
CA P 407	Inorganic Chemistry Practicals-1	4 Hrs	30 + 70	4		4	2
CA P 408	Organic Chemistry Practicals-1	4 Hrs	30 + 70	4		4	2
CA P 409	Physical Chemistry Practicals-1	4 Hrs	30 + 70	4		4	2

Total credits from 1St Semester: 21 (Hard Core-9, Soft Core-12)

2nd Semester

Course Code	Course Title	No. of Units	Evaluation IA + Exam	Teaching hrs week	Sem	Exam Hrs	Credits
CA H 451	Advanced Inorganic Chemistry	3	30 + 70	3	45	3	3
CA H 452	Advanced Organic Chemistry	3	30 + 70	3	45	3	3
CA H 453	Advanced Physical Chemistry	3	30 + 70	3	45	3	3
CA S 454 Or CA S 455	Organic Spectroscopic Techniques or Chemistry of Bio-molecules	3 3	30 + 70 30 + 70	3 3	36 36	3 3	3
CA E 456	Environmental, Electro- and Surface Chemistry	3	30 + 70	3	36	3	3

CA P 457	Inorganic Chemistry Practicals-II	4 Hrs	30 + 70	4	4	2
CA P 458	Organic Chemistry Practicals-II	4 Hrs	30 + 70	4	4	2
CA P 459	Physical Chemistry Practicals-II	4 Hrs	30 + 70	4	4	2

Total credits from 2nd Semester: 21 (Hard Core-9, Soft Core-9, Elective-3)

3rd Semester

Course Code	Course Title	No. of Units	Evaluation IA + Exam	Teaching hrs week Sem	Exam Hrs.	Credits
CA H 501	Principles of Analytical Chemistry	3	30 + 70	3 45	3	3
CA H 502	Bioanalytical & Radiochemical Techniques	3	30 + 70	3 45	3	3
CA H 503	Chromatographic Separation Techniques	3	30 + 70	3 45	3	3
CA S 504 Or CA S 505	Thermoanalytical Techniques Or Analytical Chemistry of Polymers	3 3	30 + 70 30 + 70	3 36	3	3
CA E 506	Analytical & Green Chemistry	3	30 + 70	3 36	3	3
CA P 507	Analytical Chemistry Practicals-III	6 Hrs	30 + 70	6	6	3
CA P 508	Analytical Chemistry Practicals - IV	6 Hrs	30 + 70	6	6	3
CA P 509	Analytical Chemistry Practicals - V	6 Hrs	30 + 70	6	--	3

Total Credits from 3rd Semester = 24 (Hard Core-18, Soft Core-3 and Elective-3)

4th Semester

Course Code	Course Title	No. of Units	Evaluation IA + Exam	Teaching hrs week Sem	Exam Hrs	Credits
CA H 551	Applied Analysis	3	30 + 70	3 45	3	3
CA H 552	Optical Methods of Analysis	3	30 + 70	3 45	3	3
CA H 553	Process Analytical Chemistry	3	30 + 70	3 45	3	3
CA H 554 Or	Environmental Chemistry Or	3	30 + 70	3 36	3	3

CA S 555	Pharmacokinetics & Nanimaterials					
CA S 555	Separation Techniques	3 3	30 + 70	3 36 3 36	3	3
CA P 557	Analytical Chemistry Practicals-VI	6 hrs	30 + 70	6	6	3
AC P 558	Analytical Chemistry Practicals-VII	6 Hrs	30 + 70	6	6	3
CA P 559	Project Work & Dissertation	8 Hrs	30 + 70	8		4

Total Credits from 4th Semester = 25 (Hard Core-18, Soft Core-6 + Seminar- 1)

Total Credits : 21+21+24+25 = 91.

Question Paper Setting:

A) BASIS FOR INTERNAL ASSESSMENT: Internal assessment marks in theory papers shall be based on two tests. The tests may be conducted 8 and 14 weeks after the start of a semester. Average of two test marks will be considered as internal assessment marks. Practical internal assessment marks shall be based on test and records. 20 marks for experiment and 10 marks for record. The practical tests may be conducted 12 weeks after the start of a semester. Internal Assessment marks on Project work-Dissertation is based on Two seminars of 45 minutes duration each carrying 15 marks. The Seminar is to be delivered in 3rd semester on the subject and 4th semester on their project work.

B) **THEORY QUESTION PAPERS PATTER**N: The Syllabus of each hard core course shall be grouped into units of 15 teaching hours and that of soft core and open Elective shall be of 12 teaching hours. All the papers shall contain three units each. Question Papers in all the four semesters hall consist of Two Parts A and B. Part A is shall contain Nine (09) very short answer objective type questions carrying 2 marks each drawn from all the Three units of the syllabus. All the nine subdivisions are to be answered. Part B shall contain Six (06) brief and/or long answer questions carrying 13 marks each drawn from all the Three units of the syllabus (2 questions per unit). There may be a maximum of three sub-divisions per question, carrying 3 or more marks per sub-division. Four (04) out of Six (06) questions are to be answered.

C) **PRACTICAL EXAMINATION PATTERN**

Practical Examination course papers out of 70 marks 15 marks shall be allotted for Viva voce and 55 marks for practical proper. In the 4th semester there shall project work/dissertation in lieu of one of the practicals for all the programmes (Chemistry, Applied Chemistry, Organic Chemistry and Analytical Chemistry) consisting of 70 marks. . The Project work may be conducted either in the department or in an Institution or Industry. Project report shall be valued for 70 marks.

FIRST SEMESTER

CA H 401 : INORGANIC CHEMISTRY

UNIT- I: **[15 Hours]**

Ionic bond: Properties of ionic substances, coordination number of an ion, structures of crystal lattices- NaCl, CsCl, ZnS and rutile. Lattice energy- Born Lande equation, Born-Haber cycle, Uses of Born-Haber type of calculations. Ionic radii, methods of determining ionic radii, factors affecting ionic radii, radius ratio rule, covalent character in ionic bonds, hydration energy and solubility of ionic solids.

Covalent bond: valence bond theory, resonance, hybridisation, Bent's rules and energetics of hybridization, Deduction of molecular shapes – VSEPR theory.

M.O.theory, application to homo- and hetero-diatomic and -triatomic molecules.

UNIT -II: **[15 Hours]**

Alkali and alkaline earth metal complexes of crown ethers, cryptands and calixarenes and their biological significance.

Halogens and Noble gas chemistry –interhalogens, psuedohalogens, polyhalide ions, oxyhalogen species, xenon oxides and fluorides. Oxy- and peroxy acids of N, P and S.

Graphitic compounds, carbides, pure silicon, silica and silicates, zeolites.

HSAB concept. super acids. Reactions in non-aqueous media: Liquid ammonia, anhydrous sulphuric acid, glacial acetic acid, anhydrous HF, bromine trifluoride, liquid sulphur dioxide and dinitrogen tetroxide. Reactions in molten salts.

UNIT- III: **[15 Hours]**

Precipitation phenomena: precipitation from homogeneous solutions, organic precipitants in inorganic analysis. Solvent extraction of metal ions, nature of extractant, distribution law, partition coefficients, types of extractions and applications.

Theories of redox indicators, titration curves, feasibility of redox titrations.

Chelometric titrations- titration curves with EDTA, feasibility of EDTA titrations, indicators for chelometric titrations, selective masking and demasking techniques, industrial applications of masking.

Sampling techniques, preparation of samples for analysis. Nature of errors, statistical treatment of errors, the t- and F-tests, significant figures, rejection of data.

References:

1. J.E Huheey, Keiter, Keiter and Medhi: Inorganic Chemistry (4th ed.), Pearson Education, 2006.

2.Shriver, Atkins and Langford : Inorganic Chemistry (3rd edn.) OUP, 1999.

3.J.D.Lee: Concise Inorganic Chemistry, (5th edn.) Blackwell Science, 2000.

4.B.E.Douglas, D.McDaniel & A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001

5.W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.

6.R.A.Day and A.L. Underwood : Quantitative Analysis, 5th Ed. (Prentice Hall, India), 1998.

CA H 402 : ORGANIC CHEMISTRY

UNIT–I: **[15 Hours]**

Bonding in organic systems: Theories of bonding-Valence and molecular orbital approaches. Resonance, hyper-conjugation and tautomerism, Huckel molecular orbital theory and its application to simple □ systems- ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl, heptatrienyl systems. Calculation of the total □ energy and M.O. coefficients of the systems. 5 hrs

Aromaticity: Concept of aromaticity, Huckel's rule, Polygon rule, Homo-aromatic, non-aromatic and anti-aromatic systems. Aromaticity in benzenoid and non-benzenoid molecules. Annulenes & hetero-annulenes. Physical methods to study aromaticity-UV, IR &^{1}H NMR. 4 hrs

Bonds weaker than covalent: Addition compounds, crown ether complexes, cryptands, inclusion compounds, catenanes, fluxional molecules. 3 hrs

Structure and reactivity: Effects of hydrogen bonding, resonance, inductive and hyperconjugation on strengths of acids and bases. 3 hrs

UNIT-II: **[15 Hours]**

Methods of Determining Reaction Mechanism: Kinetic and non-kinetic methods, Identification of products, detection of intermediates, isotopic labeling, stereochemical evidences, cross-over experiments, Limitation of reactions, kinetic evidences and kinetic isotopic effects. 5 hrs

Reaction Intermediates: Generation, structure, stability, reactivity, detection, trapping and reactions of classical and non-classical carbocations, carbanions, free radicals, carbenes, nitrenes and arynes. Singlet oxygen-generation and reactions with organic molecules. 5 hrs

Aliphatic Nucleophilic Substitution Reactions: Mechanism and scope of aliphatic nucleophilic substitution reactions-S_N1, S_N2 and S_Ni. Stereochemistry of nucleophilic substitution reactions, allylic nucleophilic substitution reactions, Walden inversion, neighbouring group participation & anchimeric assistance. Factors influencing the rates of nucleophilic substitution reactions. 5 hrs

UNIT-III: Stereochemistry [15 Hours]

Optical Isomerism: Conformation and configuration of molecules, projection formulae, Fischer, Saw-horse, Newman and Flying wedge representations.Interconversion of these formulae. Absolute configuration (D,L) and (R,S) systems. Elements of symmetry, Psedoassymmetric centres, chirality, molecules with more than one chiral centre, threo and erythro isomers, methods of resolution, stereospecific and stereoselective synthesis, asymmetric synthesis, Cram's and Prelog's rules. Optical activity in the absence of chiral carbon-biphenyls, allenes and spiranes. Conformational analysis of cycloalkanes and decalins. Effect of conformation on reactivity. Acyclic & cyclic systems-Substituted cyclohexanes, cyclohexanones, cyclohexanols, Curtain-Hammet Principle. Stereochemistry of compounds containing nitrogen, sulphur and phosphorus. 12 hrs

Geometrical Isomerism: Cis-trans isomerism resulting from double bonds, monocyclic compounds & fused ring systems. E,Z-notations, determination of configuration of geometrical isomers, syn & anti isomers. 3 hrs

References:

1.Organic Chemistry-P.Y.Bruice (Pearson Education Pvt. Ltd.,New Delhi),2002.
2.Stereochemistry,Conformation and Mechanism-P.S.Kalsi (Wiley Eastern,New Delhi)1993.
3.Stereochemistry of Carbon Compounds-E.L.Eliel (Tata McGraw Hill, New. Delhi) 1994.
4.Advanced Organic Chemistry-Reactions, mechanisms & structure-J.March (Wiley, NY)2000.
5.Organic Chemistry-Vol. -1,2 &3-Mukherji, Singh and Kapoor. (Wiley Eastern,) 1994.
6.A guide book of mechanisms in Organic Chemistry-P.Sykes (Orient- Longman) 1985.
7.Organic Chemistry-R.T. Morrison and R.N. Boyd (Prentice Hall, New Delhi) 1994.
8.Organic Chemistry 4th Edn.–S.H. Pine et al (McGraw-Hill, London) 1987.
9.Advanced Organic Chemistry- R.A. Carey and R.J. Sundberg (Plenum, New York)1990.
10.Modern Concepts of Advanced Organic Chemistry-R.P. Narein (Vikas, Delhi) 1997.
11.A Text book of Organic Chemistry-Tewari, Vishnoi and Mehrotra (Vikas, New Delhi)1998.
12.A Text book of Organic Chemistry-3rd Edn.-R.K. Bansal, (New Age, New Delhi) 1997.
13.Organic Chemistry-3rd Edn- F.A. Carey (Tata McGraw Hill, New Delhi) 1996.
14.Stereochemistry by K. Mislow.
15. Organic Chemistry-H. Pine (Hendrickson, Cram and Hammond,Mc Graw Hill, New York) 1987.
16. Organic Chemistry-I.L. Finar (ELBS Longmann, Vol. I) 1984.

CA H 403 : PHYSICAL CHEMISTRY

UNIT-I: Catalysis [15hours]

Catalysis: Homogeneous Catalysis – equilibrium and steady state treatments, activation energies of catalysed reactions. Acid - base catalysis (general and specific), protolytic and prototropic mechanisms, catalytic activity and acid strength measurements. Kinetics of enzyme catalysed mechanisms – Michaelis – Menten mechanism. Effect of pH, temperature and inhibitors. 6hrs.

Acidity functions: Hammett acidity function, Zucker – Hammett hypothesis, and Bunnett hypothesis. 2hrs

Surface Chemistry: A review of adsorption isotherms, uni- and bi- molecular reactions. Multilayer adsorption: BET equation – application in surface area determination. Harkin – Jura equation and application. Semiconductor catalysis, n- & p- type. Mechanism of surface reactions. Langmuir – Hinshelwood and Langmuir Rideal mechanisms.7hrs

UNIT – II [15 hours]

Chemical Kinetics:

Composite reactions: Rate equation for composite reaction mechanisms (simultaneous and consecutive reactions, steady state treatment, rate determining steps and microscopic reversibility), Chain reactions (hydrogen-halogen reactions with comparison). Auto catalytic reactions(Hydrogen-Oxygen reaction) and Oscillatory reactions. 6hrs.

Reactions in solution: Solvent effects on the reaction rates, Factors determining reaction rates in solution, reaction between ions (effect of dielectric constant and ionic strength), substitution and correlation effects (Hammet and Taft equations-linear free energy relations.) Ion-dipole and dipole-dipole reactions (Pre exp factors and influence of ionic strength) and diffusion controlled reactions. 4 hrs.

Fast reactions-Introduction, Study of fast reactions by-flow, relaxation, molecular beam, and spectroscopic and analytical methods 3hrs.

Theory of reaction rates- Temperature dependence and the Arrhenius theory of reaction rates, colision theory of bimolecular reactions, its importance and limitations. Introduction to transition state theory. 2hrs.

UNIT-III : [15hours]

Electrochemistry of solutions: Ionic atmosphere-introduction, derivation and its effect on the theory of conductivity. Walden`s rule. Debye-Huckel limiting law (DHL), its modification and verification. Bjerrum theory of ion association, triple ion formation and its significance. 4hrs.

Corrosion: Introduction, Importance and principles, Forms of corrosion (Galvanic, Atmospheric, stress, microbial and soil). Techniques of Corrosion rate measurement (instrumental and non-instrumental). EMF series & Galvanic series and their limitations. Thermodynamics (Pourbaix diagram). Concept of mixed potential theory and its importance in terms of Kinetics (Tafel and Evans diagram), effect of oxidizer and passivity of corrosion. Protection against corrosion (Design improvement, Anodic and cathodic protection, inhibitors, coating). 6 hrs.

Analytical Applications of Electrochemistry -Principles and Applications of Polarography, Cyclic voltammetry, Coulometry, Amperometry and chrono systems. 5hrs.

References

1. Chemical Kinetics, K. J. Laidler, Pearson Education, Anand Sons(India) 3rd ed., 2008.
2. Fundamentals of Chemical Kinetics, M.R.Wright, Harwood Publishing, Chichesrer, 1999.
3. Kinetics & Mechanisms of Chemical Transformations, J Rajaram & J C Kuriacose, Macmillan, Delhi,42007.
4. Chemical &Electrochemical Energy Systems, R. Narayan & B. Viswanathan (University Press), 1998.
5. Industrial Electrochemistry, D. Peltcher & F. C. Walsh (Chapman & Hall)1990.
6. Principles and Applications of Electrochemistry–Crow (Chapman hall, New York) 2014
7. An Introduction to metallic corrosion and its prevention-Raj Narayan (Oxford-IBH, New Delhi), 1983.
8. Electrochemistry and Corrosion Science-Nebtor Ferez (Springer Pvt.Ltd.), Delhi, 2010.
9. Instrumental Methds of Chemical Analysis, Kudesia Sawhney, Pragati Prakasha(Meerut).

CA S 404 : SPECTROSCOPY AND ANALYTICAL TECHNIQUES

UNIT- I: [12 Hours]

Electron Spin Resonance Spectroscopy: Basic principles, hyperfine couplings, the 'g' values, factors affecting 'g' values, isotropic and anisotropic hyperfine coupling constants, Zero Field splitting and Kramer's degeneracy. Measurement techniques and Applications to simple inorganic and organic free radicals and to inorganic complexes.

NQR Spectroscopy: Quadrupolar nuclei, electric field gradient, nuclear quadrupole coupling constants, energies of quadrupolar transitions, effect of magnetic field. Applications.

Mössbauer Spectroscopy: The Mössbauer effect, chemical isomer shifts, quadrupole interactions, measurement techniques and spectrum display, application to the study of Fe^{2+} and Fe^{3+} compounds, Sn^{2+} and Sn^{4+} compounds(nature of M-L bond, coordination number and structure), detection of oxidation states and inequivalent Mössbauer atoms.

Photoelectron spectroscopy: Basic principles, valence &core binding energies, shifts in energies due to chemical forces, Photoelectron spectra of simple molecules, Auger transitions, measurement techniques. Applications.

UNIT-II [12 Hours]

Ion Exchange Chromatography : Definitions, requirements for ion-exchange resin, synthesis and types of ion-exchange resins, Principles, basic features of ion-exchange reactions, resin properties, ion-exchange capacity, resin selectivity and factors affecting the selectivity, applications of IEC in preparative, purification and recovery process. Separation of lanthanides.

Exclusion Chromatography: Theory and principle of size exclusion chromatography, experimental techniques for gel-filtration chromatography (GFC) and gel-permeation chromatography (GPC), materials for packing-factors governing column efficiency, methodology and applications.

Thermal methods: Thermogravimetric analysis, Instumentation, factors affecting the results and applications. Differential thermal analysis, simultaneous DTA-TGA curves. Differential scanning calorimetry, applications.

UNIT – III : **[12 Hours]**

Atomic Absorption Spectrometry: Principle, Theory, working of AAS instruments, analytical applications, interferences.

Emission Spectroscopy: Flame Emission Spectroscopy, plasma emission spectrometry, basic principles of flame photometry, evaluation methods in flame photometry, interferences.

Molecular Luminescence Spectroscopy: Theory of fluorescence and phosphorescence, fluorimetry in quantitative analysis, instruments, flourescence and structure, fluorescence quenching, phosphorescence method, applications in quantitative analysis.

Light-Scattering methods : Nephelometry and turbidimetry- theory, effects of concentration, particle size and wavelength on scattering, instrumentation and applications. Activation analysis.

REFERENCES :

1.A.Salahuddin Kunju and G. Krishnan: Group Theory and its Applications in Chemistry, PHI Learning, N. Delhi, 2010

2.Gurudeep Raj, Ajay Bhagi and Vinod Jain: Group Theory and Symmetry in Chemistry, 4th edn , Krishna Meetut, 2012.

3. U.C. Agarwala, H.L.Nigam, Sudha Agarwal and S.S. Kalra: Molecular Symmetry in Chemistry via Group Theory, Anne Books, N. Delhi, 2013.

4.G.D. Christian : Analytical Chemistry, (4th Ed.), (John Wiley),1986.

5. R.A.Day and A.L. Underwood : Quantitative Analysis, 5th Ed. (Prentice Hall, India), 1998.

6.H.H.Wlliard, L.L.Merrit and J.J.Dean, Instrumental methods of analysis,(7th Ed.) 1988

7. B.K.Sharma, Instrumental Methods of Chemical Analysis (Goel publishing), 2000.
8.Skoog, Holler and Nieman: Principles of Instrumental Analysis, (Harcourt Afca), 2001

CA S 405 : ENVIRONMENTAL CHEMISTRY

UNIT-I **[12 Hrs]**

Environmental segments, evolution of earth's atmosphere. Air pollution : Air pollutants, prevention and control, Green house gases and acid rain. Carbon monoxide, industrial sources and tranportation sources. SO_x- sources, ambient concentration, test methods, control techniques - scrubbing, , limestone injection process. Ozone hole and CFC's. Photochemical smog and PAN. NO_x - Sources, ambient concentration, test methods, thermodynamics and NO_x, control techniques. Particulates : Size distribution, , particulate collection - settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters. Catalytic converters for mobile sources. Bhopal gas tragedy.

UNIT-II **[12 Hrs]**

Hydrologic cycle, sources, chemistry of sea water, criteria and standards of water quality- safe drinking water, maximum contamination levels of inorganic and organic chemicals, radiological contaminants, turbidity, microbial contaminants. Public health significance and measurement of colour, turbidity, total solids, acidity, alkalinity, hardness, chloride, residual chlorine, sulphate, fluoride, phosphate and different forms of nitrogen in natural and polluted water. Chemical sources of taste and odour, treatment for their removal, sampling and monitoring techniques. Determination and significance of DO, BOD ,COD and TOC. Water purification for drinking and industrial purposes, disinfection techniques, demineralization, desalination processes and reverse osmosis .

UNIT – III [12hrs]

Toxic chemicals in the environment, impact of toxic chemicals on enzymes. Detergents- pollution aspects, eutrophication. Pesticides- pollution of surface water. Sewage and industrial effluent treatment, heavy metal pollution. Chemical speciation- biochemical effects of pesticides, insecticides, particulates, heavy metals (Hg, As, Pb, Se), carbon monoxide, nitrogen oxides, sulphur oxides, hydrocarbon, particulates, ozone, cyanide and PAN. Solid pollutants and its treatment and disposal. Radioactive waste management.

REFERENCES :

1. A.K. De : Environmental Chemistry, (Wiley Eastern).
2. S.K.Banerji : Environmental Chemistry, (Prentice Hall India), 1993.
3 S.D. Faust and O.M. Aly : Chemistry of Water Treatment, (Butterworths),1983.
4. Sawyer and McCarty, Chemistry for Environmental Engineering(McGraw Hill) 1978
5. I.Williams, Environmental Chemistry, John Wiley, 2001
6. S.M.Khopkar, Environmental Pollution Analysis, (Wiley Eastern).

CA **S 406 : Molecular Spectroscopy & Diffraction Techniques**

Unit-I **[12 hours]**

Introduction to spectroscopy, intensity of spectral lines , Natural line width and broadening, Rotational, vibrational and electronic energy levels, selection rules.

Microwave Spectroscopy- The rotation and classification of molecules, rotation spectra of diatomic and polyatomic molecules. Rigid and non-rigid rotator models. Determination of bond length, isotope effect on rotation spectra. Stark effect, nuclear and electron spin interaction. Microwave Spectrometer.

Vibration Spectroscopy: Vibration spectra of diatomic molecules - linear harmonic oscillator, vibrational energies, zero point energy, force constants & bond strengths; anharmonicity of molecular vibrations- Morse PE diagram, selection rules, fundamental, overtones and hot bands. Vibrations of polyatomic molecules- normal modes of vibrations & nature of molecular vibrations (Ex-CO_2& H_2O).

UNIT–II : **[12 hours]** Vibration-rotation spectra of diatomic and polyatomic molecules, selection rules, PQR branches. IR Spectrophotometer-Instrumentation

Raman Spectroscopy: Classical and quantum theories of Raman effect, concept of polarizability and polarizability ellipsoid. Rotational and vibrational Raman spectra, selection rules, Raman activity of vibrations, vibrational - rotational Raman spectra, selection rules, mutual exclusion principle, polarization of Raman lines. An introduction to Laser Raman Spectroscopy. Raman Spectrometer – instrumentation. Applications of IR and Raman spectroscopy in elucidation of molecular structure (Ex - H_2O, N_2O & CO_2 molecules).

Unit III **[12Hours]**

Diffraction Techniques:Introduction, production of X-ray, Bragg`s law, Laue equations, Ewald`s diagram, X-Ray diffraction experiments – diffraction of X-rays by a crystalline powder (Debye-Scherrer and flat plate camera), powder diffractometer. Interpretation of power patterns (analytical technique). Single crystal technique - :Laue and Rotation photographic methods. Moving Film method (Weissenberg method). Systematic absences. Crystalline X-ray diffractometer (4 angle), Intensities of diffracted X-rays and structural analysis, X-ray scattering atoms and molecules, Factors affecting X-ray intensities, introduction to Crystal structure analysis. 9hrs.

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Electron Diffraction: Introduction, Theory of electron diffraction, Wierl equation and its significance (qualitatively), Elucidation of structure of simple gas molecules. Structure of surfaces - (Low and high Energy Electron Diffraction, Transmission electron microscopy (TEM), SEM. Theory and applications of Neutron diffraction. Comparison between X-ray, electron and Neutron diffractions 3hrs .

References:

1.Fundamentals of Molecular Spectroscopy, Banwell & McCash (Tata McGraw Hill, New Delhi) 2007.

2. Spectroscopy, H. Kaur (Pragathi Prakashana,Meerut), 2012.

3.Spectroscopy, Donald L.Pavia (Cengage learning India Pvt.Ltd., Delhi), 2007.

4.Spectroscopy, B.K.Sharma (Goel prakashan, Meerut), 2013.

5. A Basic Course in Crystallography, JAK Tareen and TRN Kutty, University Press, Hyderabad (2001).

6. Essentials of Crystallography, M.A. Waheb, Narosa Publishing House, New Delhi (2009),

7. X-ray methods, Clive Whiston, (John Wiley & Sons, New York) 1987.

CA P 407 : INORGANIC CHEMISTRY PRACTICALS - I

1. Analysis of Hematite-insoluble residue by gravimetry and Iron by volumetry using $Ce^{4+.}$
2. Analysis of Dolomite - insoluble residue by gravimetry and Ca, Mg by complexometry.
3. Pyrolusite - Insoluble residue by gravimetry and Manganese content by oxalate method.
4. Analysis of solder - Pb and Sn by EDTA method.
5. Complexometric determination of Mn, Cu, Ni and Fe-Cr mixture
6. Hardness of water
7. Analysis of Halide Mixture - Iodide by KIO_3 and total halide by gravimetrically.
8. Colorimetric Determination of Iron by thiocyanate and Cu by aqueous ammonia.
9. Gravimetric Determinations of Mn, Ni, Mo, Pb/Cr, sulphide, thiocyanate.
10. Statistical Analysis of Data.

Reference :

1. Vogel's Text Book of Quantitative Chemical Analysis(5th Ed), G.H.Jeffrey, J.Bassette, J.Mendham and R.C.Denny, Longman, 1999.

CA P 408 : ORGANIC CHEMISTRY PRACTICALS - I

Single and two stage organic preparations

1. Electrophilic substitution reactions–Preparations of p-bromoaniline, p-nitroaniline, 2,4,6-tribromophenol and picric acid.
2. Alkylations–Preparation of nerolin and N-methyl anthranilic acid.
3. Acetylations–Preparations of □-D-glucose penta-acetate and 2-naphthyl acetate.
4. Reactions with ring formation–Preparations of 1,2,3,4–tetrahydrocarbazole, 1-phenyl-3-methyl-5-pyrazolone and 7– hydroxy-4-methyl-coumarin.
5. Diazotisation reactions–Preparations of iodo, chloro and azo compounds.
6. Dehydration reactions–Preparations of cyclohexene and succinic anhydride
7. Condensation reactions–Condensations involving diethylmalonate and ethyl aetoacetate. Claisen-Schmidt, Aldol and Perkin condensation reactions.
8. Halogenation reactions-Preparation of n-butylbromide &□,□-dibromocinnamic acid.
9. Reduction reactions–Reductions of nitro compounds and carbonyl compounds.
10. Oxidation reactions-Preparation of p-nitrobenzoic acid, p-benzoquinone and adipic acid.

References:

1. Laboratory Manual in Organic Chemistry–R. K. Bansal (New Age, New Delhi)1990.
2. Experimental Organic Chemistry–Vol. I & II–P. R. Singh et al (TMH New Delhi)1981

3. Laboratory Manual in Organic Chemistry–Dey &Sitaraman(Allied , New Delhi)1992.

4. Vogel's Text Book of Practical Organic Chemistry including Qualitative Organic

Analysis - B. S. Furniss et al., (Longman - ELBS, London), 1989.

5. Manual of Organic Chemistry - Dey and Seetharaman.

6. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III.

8. Practical Organic Chemistry - Mann & Saunders.

CA S 409 :PHYSICAL CHEMISTRY PRACTICALS - I

(**Any 12 experiments are to be carried out)**

1. (a) Determination of transport number of Cd^{2+} and SO_4^{2-} ions by EMF method.

   (b) Determination of thermodynamic parameters of a cell reaction by EMF method.

2. Determination of pK values phosphoric acid by potentiometric/pH metric method

3. Potentiometric titration of halides in mixtures (Cl^-, Br^- and I^-) with silver nitrate

4. Verification of Nernst equation for Ag^+, $Cu^{2+}$and Zn^{2+} species.

5. Determination of Solubility product and the Instability constant by potentiometric method.

6. Potentiometric determination of solubility of insoluble silver halide and the standard electrode potential using quinhydrone electrode.

7. Conductometric titrations of displacement and precipitation reactions.

8. Determination of equivalent conductance and dissociation constants of weak acid and base.

9. Determination of solubility of lead iodide at different T & hence molar heat of solution

11. Determination of hydrolysis constant of aniline hydrochloride.

11. Determination of degree of hydrolysis of CH_3COONa and NH_4Cl by conductivity method.

12. Determination of Critical Micelle concentration by conductometric method.

13. Determination of pH of buffer solutions with a pH meter & evaluation of pK_a of acids

14. Verification of Walden`s rule (relation between viscosity of a solution and the electrical conductivity.

15. Study of variation of viscosity of a liquid with temperature

16. Determination of parachor value for CH_2 group and some elements by Surface Tension method,

17. Determination of the composition of a solution by S.T measurement .

18. Determination of the Critical Micelle Concentration by surface tension/spectrophotometric measurements.

19. Determination of the composition of Zinc Ferrocyanide complex by Potentiometric titrations.

20. Determination of Specific and molar refractivity of liquids and paracor value of a species by refractometric method.

Any other relevant experiments of interest.

References:

1. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).

2. Experiments in Physical Chemistry– James and Prichard.

3. Experimental Physical Chemistry - Daniels et al.

4. Experimental Physical Chemistry-Das & Behera (Tata McGraw Hill, New Delhi)1983.

5. Advanced Practical Physical Chemistry–Yadav (1989).

6. Experiments in Physical Chemistry–J. C. Ghosh (Bharathi Bhavan)1974.

7.Practical Physical Chemistry-B Viswanathan & P.S Raghavan,(ViVa Books, New Delhi) 2005.

2nd Semester

CA H 451: ADVANCED INORGANIC CHEMISTRY

UNIT - I: **[15 Hours]**

Symmetry and Group Theory

Definitions of group, subgroup, relation between orders of a finite group and its subgroup. Conjugacy relation and classes, symmetry elements and symmetry operations, Schonflies symbols, Matrix representations of symmetry operations, products of symmetry operations, some properties of matrices and vectors, classification of molecules into point groups. Reducible and irreducible representations. The Great Orthogonality theorem (without proof), character tables. The direct product. Applications of group theory - Molecular vibrations, group theoretical selection rules for electronic transitions, for infra red and Raman spectra. Hybrid orbitals and Molecular orbitals, transformation properties of atomic orbitals.

UNIT - II: **[15 Hours]**

Chemistry of higher boranes, classification, structures and M.O. description of bonding, framework electron counting, Wade's rules, chemistry of B_5H_9, $B_{10}H_{14}$ and $B_nH_n^{2-}$. Carboranes and metallocarboranes. Cyclophosphazenes, phosphazene polymers, S-N compounds. Coordination numbers 2-10 and their geometry, crystal field theory of coordination compounds, d-orbital splittings in octahedral, square planar and tetrahedral fields, spectrochemical series, and Jahn-Teller effect.
Structural evidences for ligand field splittings – hydration, ligation and lattice energies, site preference energies. MO theory of coordination compounds- MO energy level diagrams for octahedral and tetrahedral complexes.

UNIT - III: **[15 Hours]**

Trends in oxidations states, stereochemistry and ionic sizes of metals, comparison of 3d, 4d and 5d series by taking Ti and Ni subgroups as examples. Lanthanides and actinides: electronic structure, oxidation states, extraction and separation of lanthanides, stereochemistry, spectral and magnetic properties of lanthanide and actinide complexes, lanthanide complexes as NMR shift reagents. Comparison with d-block ions.

Methods of reduction of oxide ores, Ellingham diagram, chemical and electrolytic reductions, reduction potentials, Latimer and Frost diagrams, effect of complexation on potential.

References:

1. J.E Huheey, E.A..Keiter, R.L.Keiter & O K Medhi: Inorganic Chemistry (4th edn.), Pearson, 2006.
2. Shriver, Atkins and Langford : Inorganic Chemistry (3rd edn.) OUP, 1999.
3. J.D.Lee: Concise Inorganic Chemistry, (5th edn.) Blackwell Science, 2000.
4. B.E.Douglas, D.McDaniel &A Alexander: Concepts & Models of Inorganic Chemistry, Wiley 2001
5. W.W.Porterfield: Inorganic chemistry – A Unified Approach, Elsevier, 2005.
6.N.N.Greenwood and A. Earnshaw, Chemistry of the Elements, First Edn(Pergamon Press)
7. Basallo & Johnson, Coordination Chemistry

CA H 452 : ADVANCED ORGANIC CHEMISTRY

UNIT - I: **[15 Hours]**

Aliphatic Electrophilic Substitution Reactions: Bimolecular mechanisms-S_E1, S_E2 and S_Ei mechanism. Electrophilic substitution reactions accompanied by double bond shifts. 3 hrs

Aromatic Electrophilic and Nucleophilic Substitution Reactions: Mechanism of aromatic electrophilic substitution reactions-nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, orientation and reactivity, energy profile diagram. The ortho/para ratio, ipso attack, orientation in other ring systems. Mechanism of Vilsmeir-Haack reaction, Mannich reaction, Diazonium coupling, Pechmann reaction and Fries rearrangement. Mechanisms of aromatic nucleophilic substitution reactions- S_NAr, S_N1 & aryne mechanism. Von-Richter rearrangement, Sommelet-Houser rearrangement, Smiles rearrangement. 12 hrs

UNIT- II: **[15 Hours]**

Free Radical Reactions: Types, mechanisms of free radical substitution reactions & neighbouring group assistance. Reactivity for the aliphatic and aromatic substances at a bridgehead. Reactivity of attacking radical. Effect of solvent on reactivity. Auto-oxidation, coupling of alkynes. Arylation of aromatic compounds by diazonium salts. Sandmeyer, Ullmann & Hunsidiecker reactions. 5 hrs

Elimination Reactions: Discussions of E1, E2 and E1cB mechanisms. Orientation during elimination reactions. Saytzeff and Hofmann rules. Reactivity-effects of substrate structures, attacking base, leaving group and solvent medium. 5 hrs

Pyrolytic Eliminations: Mechanisms of pyrolysis of esters of carboxylic acids. Chugaev reactions, Hofmann degradation, Cope elimination and xanthate pyrolysis. 5 hrs

UNIT- III: **[15 Hours]**

Formation and Hydrolysis of Esters: Plurality of mechanism. Mechanism of esterification reactions. Ester hydrolysis-$A_{AC}2$, $B_{AC}2$, $A_{AC}1$ & $A_{AL}1$ mechanism. Transesterification.4 hrs

Addition to Carbon-Carbon Multiple Bonds: Addition reactions involving electrophiles, nucleophiles and free radicals. Cyclic mechanisms. Orientation and stereochemistry. Addition of halogens, hydrogen halides, carboxylic acids and amines. Addition to cyclopropanes, hydroboration, Michael addition. Addition of oxygen across double bonds. 5 hrs

Addition to Carbon-Hetero Multiple Bonds: Electrophilic, nucleophilic and free radical additions to C=O and C=N systems. Addition of Grignard reagents. Reformasky reaction, aldol condensation, Knoevenagel condensation, Perkin reaction and Wittig reactions. 6 hrs

References:

1.Organic Reactions and Their Mechanisms- P.S. Kalsi (New Age, New Delhi),1996.
2.Advanced Organic Chemistry 4th Edn- J. March (Wiley, NY) 2000.
3.Organic Reaction Mechanisms- Bansal (Tata McGraw Hill, New Delhi) 1978.
4.Organic Chemistry-Vol.–I & II-Mukherji, Singh and Kapoor(Wiley Eastern, New Delhi) 1985.
5.Mechanism and Theory in Organic Chemoistry-Lowry and Richardson Harper and Row, 1987.
6. Reaction Mechanisms in Organic Chemistry-Mukherji, Singh and Kapoor (McMillan) 1978.
7. Organic Chemistry-P.Y. Bruice (Pearson Education, New Delhi) 2002.
8. Organic Reaction Mechanism-R.K. Bansal (Wiley Eastern Limited, New Delhi) 1993.
9. A Guide Book to Mechanism in Organic Chemistry-Petersykes.
10. Advanced Organic Chemistry –Carey and Sundberg, Part A & B, 3rd edition (Plenum Press, New York) 1990.
11. Organic Chemistry-I.L. Finar (ELBS Longmann, Vol. I) 1984.
12. Advanced General Organic Chemistry-S.K. Ghosh (Book and Alleied (P) Ltd) 1998.

CA H 453 : ADVANCED PHYSICAL CHEMISTRY

UNIT I: **[15hours]**

Chemical Thermodynamics:

Entropy: Physical significance, entropy change in an ideal gas. Variation of entropy with Temperature, Pressure and Volume. Entropy change in reversible and irreversible processes. Thermodynamic equations of state.

Free energy, Maxwell's relations and significance. Helmholtz's and Gibbs free energies, Gibbs – Helmholtz equation and its applications.

Nernst heat theorem : Its consequences and applications. Third law of thermodynamics – statements, applications and Comparison with Nernst Heat theorem.

Chemical affinity and thermodynamic functions. Effect of temperature and pressure on chemical equilibrium- van't Hoff reaction isochore and isotherms.

Partial molar properties: Physical significance, determination of partial molar volume and enthalpy. Chemical potential: variation of chemical potential with temperature. Gibbs – Duhem equation.

Thermodynamic functions of mixing, Gibbs – Duhem – Margules equation.

Fugacity: Relationship between fugacity and pressure. Determination of fugacity- graphical method and Lewis Randall rule.
Activity and activity coefficient: Variation of activity and fugacity with temperature and pressure. Determination of activity by vapour pressure method.

UNIT - II: Statistical and Irreversible thermodynamics [15 hours]

Statistical Thermodynamics : Thermodynamic Probability, phase space, micro and macro states, statistical weight factor, assembly, ensemble-significance, classification and comparison. Distribution laws – Boltzmann law, Maxwell-Boltzmann distribution law. Bose-Einstein and Fermi-Dirac statistics, Limit of applicability of various laws. Relationship between partition function and thermodynamic functions -Average energy, heat capacity, free energy, chemical potential. Introduction to Statistical mechanism of independent, independent and indistinguishable (non-localized) molecules or particles.
Partition function for molecular particles. .
Thermodynamic quantities in terms of partition function of particles- Evaluation of Translational, vibrational, rotational, electronic and nuclear derivations of translational, rotational, vibrational and electronic partition functions. .
Law of equipartition principle. Partition function and equilibrium constant. .
Statistical thermodynamic properties of solids (Heat capacity)- Introduction, thermal characteristics of crystalline solid, Einstein model, Debye modification. Nuclear statistics - Introduction, symmetric and nuclear spin, ortho and para nuclear states. Applications of partition function to mono atomic gases, diatomic molecules, equilibrium constant.
9hrs.**Irreversible Thermodynamics** – Introduction, Thermodynamics of irreversible processes, Entropy production-rate of entropy production. Phenomenological relations. The principle of microscopic reversibility, Onsager reciprocal relations – validity and applications (Electro kinetic, Thermoelectric phenomena). Irreversible thermodynamics of Non linear regime and biological systems. 6hrs.

UNIT III: **Quantum Chemistry [15 hours]**

Postulates of quantum Mechanics. Particle waves, its character and significance. Normalization and orthogonality of wave functions. Operators and their algebra, types and applications, operators for the dynamic variables of a system (position, linear momentum, angular momentum, Kinetic energy, potential energy and total energy) . Eigen values and Eigen functions. Quantum numbers and their characteristics. Shrodinger wave equation- significance and derivation. Statistical interpretation of ψ. 7hrs

Solution of SWE for simple systems-particle in a box (1D & 3D), particle in a ring, simple harmonic oscillator, rigid rotor, the H atom (solution of r,θ,Φ equations). Chemical Bonding in diatomics: Covalent bond-Valence bond and molecular orbital approaches with comparison.

Molecular orbital theory applied to homonuclear and heteronuclear diatomic molecules. Introduction to Huckel molecular orbital theory of conjugated systems and its applications. 8hrs

References:

1.Thermodynamics for Chemists- S Glasstone(East West press)
2.Physical Chemistry-P W Atkins.
3.Chemical Themodynamics, Rajaram and Kuriokose (East-West)Pearson, Chennai, 2013.
4. Thermodynamics, 3rd Ed., R.C. Srivastava and Subit K Saha (Prentice-Hall of India, Delhi), 2007.
5. Statistical Thermodynamics, M. C. Gupta (New ge International, Delhi) 2007.

6.Principles of Physical chemistry; B.R.Puri, L.R.Sharma and M.S.Pathania, Vishal Publishers(2014)
7.Atomic Structure and Chemical Bond , Manasa Chanda, Tata McGraw Hill Publishers(1991).
8.Quantum Chemistry, R.K.Prasad, New Age International (1991)
9.Advanced Physical Chemistry- Gurdeep R Chatwal (Goel Publishes, Meerut), 1992.
10.Introductory Quantum Chemistry – A.K.Chandra (Tata McGraw Hill) 1994.
11.Quantum Chemistry, A.B.Sannigrahi (Book and Allied Pvt.Ltd., Kolkatt), 2013.
12.Quantum Chemistry, Donald A.P (Viva Books, Delhi), 2013.

CA S 454 : ORGANIC SPECTROSCOPIC TECHNIQUES

UNIT–I: **[12 hours]**

UV/Electronic Spectroscopy: Basic principles, Chromophores, auxochromes, Instrumentation and application. Factors affecting the positions of UV bands. Electronic transitions and empirical correlations of predicting λ_{max} of organic compounds. Woodward–Fieser rules. UV absorption of aromatic compounds - effect of substituents and solvent effects. Emperical rules to calculate $\lambda_{max.}$ Application of UV spectroscopy in the structural study of organic molecules.5 hrs

IR Spectroscopy: Basic principles, Application of infrared spectroscopy in the structural study-identity by finger printing and identification of functional groups. Characteristic vibrational frequencies of common functional groups (alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines). Study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, anhydrides and acids). Factors affecting band positions and intensities such as effect of hydrogen bonding, phase and solvent on vibrational frequencies, overtones, combination bands and Fermi resonance. 7 hrs

UNIT-II: Nuclear Magnetic Resonance Spectroscopy **[12 hours]**

Theory and principle, NMR spectrometer, FT NMR and its advantages. Solvents used, chemical shift and its measurements, factors affecting chemical shift. Integration of NMR signals, spin-spin coupling, coupling constant. Shielding and deshielding. Chemical shift assignment of major functional groups, Classification (ABX, AMX, ABC, A_2B_2), spin decoupling, effects of chemical exchange, fluxional molecules, Hindered rotation through NMR spectrum, Karplus relationships (Karplus curve–variation of coupling constant with dihedral angle), double resonance techniques,

NMR shift reagents, solvent effects and Nulear Overhauser Effect. High resolution ^{1}H NMR. Applications of NMR spectroscopy in structure elucidation of simple organic and inorganic molecules. Pulse techniques in NMR, two dimensional and solid state NMR. Use of NMR in Medical diagnostics. 10 hrs

NMR of nuclei other than proton: ^{13}C chemical shift & factors affecting it. Decoupling-Noise decoupling & broad band decoupling. Off-resonanceproton decoupling-some representative examples. Introduction to ^{19}F & ^{31}P NMR. 2 hrs

UNIT-III: Mass Spectrometry [12 hours]

Basic principles, Instrumentation, interpretation of mass spectra, resolution, exact masses of nucleides, molecular ions, meta-stable ions and isotope ions. Fragmentation processes-representation of fragmentation, basic fragmentation types and rules. Factors influencing fragmentations and reaction pathways. McLafferty rearrangement. Fragmentations associated with functional groups- alkanes, alkenes, cycloalkanes, aromatic hydrocarbons, halides, alcohols, phenols, ethers, acetals, ketals, aldehydes, ketones, quinines, carboxylic acids, esters, amides, acid chlorides, nitro compounds and amines. Ion analysis, ion abundance, retro Diels-Alder fragmentation. Nitrogen rule. High resolution mass spectroscopy. 9 hrs

Composite problems involving the applications of UV, IR, ^{1}H and ^{13}C NMR and mass spectroscopic techniques. Structural elucidation of organic molecules. 3 hrs

REFERENCES:

1. Spectrometric Identification of Organic Compounds - Silverstein, Bassler & Monnill (Wiley)1981.

2. Applications of Absorption Spectroscopy of Organic Compounds-Dyer(Prentice Hall,NY) 1965.

3. Spectroscopy of Organic Compounds-3rd Ed.-P.S.Kalsi (New Age, New Delhi) 2000.

4. Analytical Chemistry-Open Learning : Mass spectrometry.

5. Spectroscopic Methods in Organic Chemistry - Williams and Fleming, TMH.

6. Spectroscopy, Donald L.Pavia (Cengage learning India Pvt.Ltd., Delhi), 2007.

7. Organic Spectroscopy-3rd ed.-W.Kemp (Pagrave Publishers, New York), 1991.

CAS 455 : ANALYTICAL AND GREEN CHEMISTRY

UNIT I: 12 Hours

Cell Structure and Functions: Structure of prokaryotic and eukaryotic cells, intra ellular organelles and their functions, comparison of animal and plant cells. Overview of metabolic processes – catabolism and anabolism. ATP- the biological energy currency. Origin of life – unique properties of carbon, chemical evolution and rise of living systems.

Lipids: Fatty acids, essential fatty acids, structure and function of triacylglycerides, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins.

Lipoprotiens: composition and function, role in atherosclerosis, properties of lipid aggregates, micelles, bilayers, liposomes and their biological functions. Biological membranes- Fluid mosaic model of membrane structure. Lipid metabolism(□-oxidation of fatty acids).

Unit II: 12 Hours

Enzymes: Introduction**,** Classification, Enzyme substrate complex formation models: Lock and Key model, Host-Guest and Induced- Fit model. Factors affecting enzyme activity (pH, temperature), enzyme inhibition (reversible and irreversible) and immobilised enzymes. Examples of some typical enzyme mechanisms for Triose phosphate isomerase, α- Carboxy peptidase-A and Ribonuclease. Enzymatic synthesis of α-amino acids and peptides. Transformations of lipases and esterases. Kinetic resolutions of catboxylic acids, esters and alcohols-Transesterification. Enzymatic synthesis of α-amino acids and peptides. Transformations of lipases and esterases.

Coenzymes 12 Hours

Introduction. Co factors - cosubstrates - prosthetic groups. Classification-Vitamin derived coenzymes and metabolite coenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate (TPP), pyridoxal phosphate (PLP), oxidized and reduced forms of nicotinamide adenosine dinucleotide / their phosphates (NAD, NADH, $NADP^+$, NADPH), Flavin adenine nucleotide (FAD, FADH2), Flavin mononucleotide (FMN, FMNH2) and tetrahydrofolate. Adenosine triphosphate (ATP) and adenosine diphosphate (ADP). Mechanism of reactions catalyzed by the above coenzymes.

References:

1. Principles of Biochemistry – A L Lehninger, Worth Publishers.
2. Biochemistry – L Stryer, W H Freeman.
3. Biochemistry – J David Rawn and Neil Patters.
4. Biochemistry – Voet and Voet, John Wiley.
5. Outlines of Biochemistry – E E Conn and P K Stumpf. John Wiley.
6. Enzyme structure and mechanism - Fersht and Freeman
7. Outlines of Biochemistry - Conn and Stumpf
8. Principles of Biochemistry - Horton & others.
9. Bioorganic chemistry - A chemical approach to enzyme action - Herman Dugas and Christopher Penney.

CA E 456 : ENVIRONMENTAL, ELECTRO AND POLYMER CHEMISTRY

UNIT-I: [12 Hours]

Environmental segments, evolution of earth's atmosphere. Air pollution : Air pollutants, prevention and control, Green house gases and acid rain. Carbon monoxide, industrial sources and transportation sources. SO_x- sources, ambient concentration, test methods, control techniques - scrubbing, limestone injection process. Ozone hole and CFC's. Photochemical smog and PAN. NO_x - Sources, ambient concentration, test methods, thermodynamics and NO_x, control techniques. Particulates : Size distribution, particulate collection - settling chambers, centrifugal separators, wet scrubbers, electrostatic precipitators & fabric filters. Catalytic converters for mobile sources. Bhopal gas tragedy.

UNIT-II [12 hrs]

Corrosion - Introduction, consequence, types, prevention and measurement. Conventional sources of energy, limitations, Importance of storage, Battery-Electrodes, Cell, battery Brief account of primary, secondary, lithium battery and fuel cells. Semiconductor electrodes and Solar energy system. .

Introduction to bioelectrochemistry, electrochemical communication in biological organisms. Theory and applications of Electroplating and electroless plating. 7hrs .

Reaction Kinetics-Theory and applications of different types of reactions- Oscillatory, chain reaction, branched chain reaction. .

Energy of activation and thermodynamic parameters, Collision theory of reaction rates, limitations and basics of transition state theory. 5 hrs

UNIT- III [12 hrs]

Polymers:

Introduction- Basic concepts and classification of polymers, Molecular weight and its distribution, Chemistry of polymerization- Step, chain, Coordination, Copolymerization. Polymerization techniques- bulk, solution, suspension, emulsion, poly-condensation, solid and gas phase polymerization.

Chemical and geometrical structure of polymer molecules, Structure property relationship- Physical, Thermal and mechanical properties 6hrs

Synthesis, properties, structural features and applications of some important commercial polymers (PE, PP,PS, PVC, PMMA, PET, Nylon-6,Nylon-6,6) , Engineering polymers (Kevlar, Nomex, ABS, PC, Teflon). Applications of polymers in separations: reverse osmosis, ultra and nano-filtration. Applications in electronics- conducting polymers and electronic shielding, Applications of polymers in medicine.

Management of plastics in environment- recycling, incineration and biodegradation. -6hrs

References:
1. A.K. De : Environmental Chemistry, (Wiley Eastern).
2. S.K.Banerji : Environmental Chemistry, (Prentice Hall India), 1993.
3. Sawyer and McCarty, Chemistry for Environmental Engineering(McGraw Hill) 1978.
4. An Introduction to metallic corrosion and its prevention-Raj Narayan (Oxford-IBH, New Delhi), 1983.
5.Chemical & Electrochemical Energy Systems, R. Narayan & B. Viswanathan (University Press), 1998.
6. Industrial Electrochemistry, D. Peltcher & F. C. Walsh (Chapman & Hall)1990.
7. F.W. Billmeyer, Text book of Polymer science, 3rd Ednn, A Wiley- Interscience Publication, New York, 2005
8.. V.R. Gowariker, Polymer Science, New Age International (P) Ltd., New Delhi, 2012
9. R.W. Dyson, Specialty Polymers, Chapman and Hall, New York, 1987
10. J.R. Fried, Polymer Science and Technology, Prentice Hall of India Pvt. Ltd., New Delhi, 1999
11. P. Ghosh, Polymer Science and Technology, Tata - McGraw Hill, New Delhi, 1995

CA P 457: INORGANIC CHEMISTRY PRACTICALS-II

Qualitative Analysis of mixtures of Inorganic Salts containing 3 cations and 2 anions (1 less common metal ions like Tl, W, Mo, V, Zr, Th, U, Ce, Ti and Li to be included among anions organic acid radicals, phosphate, borate and fluoride separation included).

References:

1. Vogel's Text Book of Quantitative Chemical Analysis (5^{th} Ed), G. H. Jeffrey, J. Bassette, J.Mendham and R. C. Denny, Longman, 1999

2. Vogel's Qualitative Inorganic Analysis (7^{th} Ed), G. Svehla, Longman (2001).

CA P 458 : ORGANIC CHEMISTRY PRACTICALS-II

Separation and systematic qualitative analysis of binary mixtures of organic compounds containing both mono and bifunctional groups and preparation of suitable derivatives.

References:

1.Practical Organic Chemistry-F .G. Mann and B. C. Saunders (ELBS, England), 2001.

2. Practical Organic Chemistry - A. I. Vogel (Longman-ELBS, England), 1971.

3. Experimental Organic Chemistry–Vol.I&II Singh et al(TMH, New Delhi)1981.

4. Semimicro Qualitative Organic Analysis–Cheronis etal Wiley-Eastern, New Delhi) 1964.

5. Vogel's Text Book of Practical Organic Chemistry Including Qualitative Organic Analysis- B. S. Furniss *et al* (Longman-ELBS, England), 1978.

6. Manual of Organic Chemistry - Dey and Seetharaman.

7. Modern Experimental Organic Chemistry-John H. Miller and E.F. Neugil.

CA P 459 :PHYSICAL CHEMISTRY PRACTICALS- II

(At least 12 experiments are to be carried out)

1. Determination of cryoscopic constants of solvents and molecular weight of non volatile substances by thermal method.

2. Determination of degree of dissociation, Vant Hoff factor and molecular weight of an electrolyte by cryoscopy method using copper calorimeter/Dewar flask..

3. Heat of solution of a sparingly soluble compound in water by solubility method.

4. Phase diagram of two component systems by thermal analysis.

5. Phase diagram of three component system (a) 3 liquids with single binodal curve, and b) two liquids and one solid

6. Kinetics of acid catalyzed hydrolysis of methyl acetate and determination of (a) order and rate constant and (b) Energy of activation.

7. Determination of a) Energy of activation & b) rate constant for the First and second order kinetics of reaction between potassium persulphate and potassium iodide.

8. Kinetics of sodium formate – iodine reaction.

9. Determination of the latent heat of evaporation of carbon tetrachloride.

10. Preparation of colloidal solutions.
11. Verification of F & L adsorption isotherms for acetic acid on activated charcoal.

12. To study the adsorption of iodine on charcoal from alcoholic solution.

13. To study the effects of gelatin solution on the precipitation values.

14. Comparison of detergent action of detergents and determination of interfacial tension.

15. Thermodynamic prediction and measurement of the solubility of naphthalene in benzene.
16. Study of association of benzoic acid in benzene/toluene.

Any other relevant experiments of interest.

References:-

1. Practical Physical Chemistry- B Viswanathan & P.S Raghavan,(ViVa Books, Delhi) 2005.
2. Findlay's Practical Physical Chemistry- B. P. Levitt (Longman, London).
3. Experiments in Physical Chemistry– James and Prichard.
4. Experimental Physical Chemistry - Daniels et al.
4. Experimental Physical Chemistry-Das & Behera (Tata McGraw Hill, New Delhi)1983.
5. Advanced Practical Physical Chemistry–Yadav (1989).
6. Experiments in Physical Chemistry–J. C. Ghosh (Bharathi Bhavan)1974.